

Correlation functions in the factorization approach of nonextensive quantum statistics

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We study the long range behavior of a gas whose partition function depends on a parameter q and it has been claimed to be a good approximation to the partition function proposed in the formulation of nonextensive statistical mechanics. We compare our results, at large temperatures and at the critical point, with the case of Boltzmann-Gibbs thermodynamics for the case of a Bose-Einstein gas. In particular, we find that for all temperatures the long range correlations in a Bose gas decrease when the value of q departs from the standard value $q = 1$.

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I. INTRODUCTION

The formulation of nonextensive statistical mechanics [1] has raised numerous questions regarding its relevance to systems with long range interactions, long range microscopic memory, or multifractal properties [2]. This formalism can also be understood as a generalization of Boltzmann-Gibbs statistics, opening the possibility to get a theoretical insight on the thermodynamics of systems whose behavior depart from Boltzmann-Gibbs statistical mechanics. The generalized entropy

$$S_q = \frac{k}{q-1} \left(1 - \sum_R p_R^q \right), \quad (1)$$

is a function of the probability p_R for the ensemble to be in the state R and a real parameter q . Equation (1) becomes the Shannon entropy as $q \rightarrow 1$. In addition, Tsallis' entropy shares all the properties of the Shannon entropy except that of additivity. Considering two independent systems Σ and Σ' , the entropy S_q satisfies the pseudoadditivity property

$$\frac{S_q^{\Sigma \cup \Sigma'}}{k} = \frac{S_q^{\Sigma}}{k} + \frac{S_q^{\Sigma'}}{k} + (1-q) \frac{S_q^{\Sigma}}{k} \frac{S_q^{\Sigma'}}{k}. \quad (2)$$

The probability distribution that results from extremizing the entropy with the constraints

$$\sum_R p_R = 1, \quad (3)$$

and

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$$\langle E \rangle = \sum_R p_R^q E_R, \quad (4)$$

is given by the equation

$$p_R = \frac{[1 + \beta(q-1)(E_R - \mu N)]^{1/(1-q)}}{Z_q}, \quad (5)$$

with the partition function

$$Z_q = \sum_R [1 + \beta(q-1)(E_R - \mu N)]^{1/(1-q)}, \quad (6)$$

and the total energy $E_R = \sum_j n_j \varepsilon_j$. Due to the mathematical complexity of the partition function in Equation (6), it has been necessary to study the validity of certain approximation procedures. Thus, the study of the consequences of nonextensivity has been mainly focused on either assuming a value of $q \approx 1$ [3] or by approximating the partition function in Eq. (6) by a factorized partition function [4]

$$Z = \prod_{j=0} \sum_{n_j=0} [1 + \beta(q-1)n_j(\varepsilon_j - \mu)]^{1/(q-1)}. \quad (7)$$

The factorization approach has been shown [5] to be a good approximation to Tsallis partition function outside certain narrow temperature interval that shifts to higher values of T when the number of energy levels increases. An application to the Ising model and black body radiation can be found in Refs. [6] and [7] respectively. In this approximation the average number of particles with energy ε is given by the function

$$\langle n \rangle = \frac{1}{[1 + \beta(q-1)(\varepsilon - \mu)]^{1/(q-1)} + a}, \quad (8)$$

where $a = 0, -1, +1$ for Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac cases respectively. It is important to remark that the function $\langle n \rangle$ has also been obtained [8] by extremizing the entropy related to the generalized dimensions of a fractal set. It has been also pointed out [10] that nonextensive thermodynamics could also be understood in terms of q -deformations and possibly with the theory of quantum groups. Along this line of work, in Ref. [9] we made a study of the basic thermodynamics that result from the particle distribution functions in Eq. (8) for classical and quantum gases. In that article we shown that the high temperature behavior is consistent with the thermodynamical limit provided that the internal energy is calculated according to the equation

$$\langle U \rangle = \frac{4\pi V}{h^3} \int_0^\infty \frac{p^2}{2m} \langle n(p) \rangle^q p^2 dp. \quad (9)$$

By introducing the usual creation and annihilation operator formalism we found that the boson hamiltonian that leads to the particle distribution, for $a = -1$, in Eq.(8) is written as

$$\hat{K} = \sum_{j=0} (\varepsilon_j - \mu) \bar{\phi}_j \phi_j, \quad (10)$$

where the operator ϕ_j and its adjoint $\hat{\phi}_j$ satisfy a deformed boson algebra. However, a comparison of the heat capacity and entropy functions, in Ref. [9], for systems with a particle distribution function as given by Eq. (8) with those for

Bose and Fermi gases described by quantum group invariant hamiltonians [11] shows that nonextensivity is unrelated to quantum group invariance.

In this paper we calculate the correlation function for boson systems with a particle distribution function as given by Eq. (8). Our main motivation in studying this system is twofold. First, it is of theoretical interest to study a thermodynamics system which obeys a statistical mechanics that generalizes Boltzmann-Gibbs statistics. Second, a calculation of the correlation functions will give us an insight on the long-range behavior dependence of these thermodynamical systems on the parameter q . Our calculations will show in a concrete fashion the relation between q and long-range behavior, and will indicate whether the thermodynamics resulting from Eq. (8), proposed in Ref. [4], has the long range behavior expected to be present in nonextensive thermodynamics. In Sec. II we calculate the correlation function for $q \neq 1$, and discuss the results for some particular values of this parameter. We specialize our discussion to the behavior near the critical temperature T_c and at large values of T . In Sec. III we summarize our results.

II. CORRELATION FUNCTIONS

According to our previous work [9], the parameter q cannot be any real number but its values are restricted to those such that $1/(q-1)$ is an integer. In addition, the thermodynamic functions are well defined only in the interval $1 \leq q \leq 1.5$. The correlation for a Bose gas with particle distribution according to Eq.(8) is given by

$$G(\mathbf{R}) = \frac{1}{V} \sum_{\mathbf{k}} \frac{e^{i\mathbf{k} \cdot \mathbf{R}}}{[1 + \beta(q-1)(\varepsilon - \mu)]^{1/(q-1)} - 1}, \quad (11)$$

As usual, this summation can be approximated by an integration over \mathbf{k} , leading after integration over the angles for $d = 3$ to the equation

$$G(\mathbf{R}) = \frac{\langle N_0 \rangle}{V} + \frac{2}{\pi^{1/4} R^{1/2} (\lambda \sqrt{q-1})^{5/2}} \int_0^\infty x^{3/2} \sum_{j=1}^\infty [1 + \alpha(q-1) + x^2]^{-j/(q-1)} J_{1/2} \left(2\pi^{1/2} R x / \lambda \sqrt{q-1} \right) dx, \quad (12)$$

where the new variable $x^2 = \beta(q-1)k^2\hbar^2/2m$ and, as usual, $\alpha = -\beta\mu$ and λ is the thermal wavelength. The integral in Eq. (12) is tabulated [12]

$$\int_0^\infty \frac{J_\nu(bx)}{(x^2 + c^2)^{\mu+1}} x^{\nu+1} dx = \frac{c^{\nu-\mu} b^\mu}{2^\mu \Gamma(\mu+1)} K_{\nu-\mu}(cb), \quad (13)$$

where $-1 < \text{Re } \nu < \text{Re}(2\mu + 3/2)$, $c > 0$ and $b > 0$. It is simple to check that all these inequalities are satisfied for all the allowed values of q in the interval $1 \leq q \leq 1.5$. Defining a length parameter $\chi < \lambda$

$$\chi = \frac{\lambda}{2\sqrt{\pi}} \sqrt{\frac{q-1}{1 + \alpha(q-1)}}, \quad (14)$$

and by use of the integral representation

$$K_\nu(zx) = \frac{\Gamma(\nu + 1/2)}{x^\nu \Gamma(1/2)} (2z)^\nu \int_0^\infty \frac{\cos(xt)}{(t^2 + z^2)^{\nu+1/2}} dt, \quad (15)$$

the correlation function reduces to the expression

$$G(\mathbf{R}) = \frac{1}{\pi R \lambda^2 (q-1)} \int_0^\infty \cos(t) \sum_{n=1} \left[\frac{(R/\chi)^2}{(1 + \alpha(q-1))(t^2 + (R/\chi)^2)} \right]^{n/(q-1)-1} dt. \quad (16)$$

Once we perform the summation we get a set of integrals in terms of elementary functions. These integrals are all tabulated [13] and the correlation function for some values of q follows

$$G(\mathbf{R}) = \begin{cases} (1/R\lambda^2) \left[e^{-R/\xi} - e^{-\sqrt{(R/\xi)^2 + 32\pi(R/\lambda)^2}} - 2e^{-A'} \sin(B') \right] & \text{for } q = 5/4 \\ (1/R\lambda^2) \left[e^{-R/\xi} - e^{-A} \cos(B) - \sqrt{3}e^{-A} \sin(B) \right] & \text{for } q = 4/3, \\ (1/R\lambda^2) \left[e^{-R/\xi} - e^{-\sqrt{(R/\xi)^2 + 16\pi(R/\lambda)^2}} \right] & \text{for } q = 3/2 \end{cases} \quad (17)$$

where $\xi = \lambda/2\sqrt{\pi\alpha}$ is the correlation length and the exponents

$$\begin{aligned} A^2 &= 12\pi(R/\lambda)^2 \left[(1/2)\sqrt{(3/2 + \alpha/3)^2 + (3/4)} + (3/2 + \alpha/3) \right] \\ B^2 &= 12\pi(R/\lambda)^2 \left[(1/2)\sqrt{(3/2 + \alpha/3)^2 + (3/4)} - (3/2 + \alpha/3) \right] \\ A'^2 &= 16\pi(R/\lambda)^2 \left[(1/2)\sqrt{(1 + \alpha/4)^2 + 1} + (1 + \alpha/4) \right] \\ B'^2 &= 16\pi(R/\lambda)^2 \left[(1/2)\sqrt{(1 + \alpha/4)^2 + 1} - (1 + \alpha/4) \right] \end{aligned}$$

From these equations it is clear that the correlation functions for $q \neq 1$ have a leading term

$$G(\mathbf{R}) \approx (1/R\lambda^2)e^{-R/\xi}, \quad (18)$$

minus some smaller additional terms which are absent in the Bose-Einstein case.

A. Correlation length

In order to compare these correlation functions with the standard correlation function $G_{BE}(\mathbf{R})$ we first look at the case of high temperature $T \gg T_c$. Although Eq. (18) has the same functional relation than

$$G_{BE}(\mathbf{R}) \approx (1/R\lambda^2)e^{-R/\xi_{BE}}, \quad (19)$$

the parameter α is the function [9]

$$\alpha = \frac{1}{q-1} \left[-1 + \left(\frac{-2}{\sqrt{\pi}\langle n \rangle (q-1)^{3/2} \lambda^3} S_2(q) \right)^{2(q-1)/(5-3q)} \right], \quad (20)$$

with

$$S_2(q) = \frac{1}{3/2 - 1/(q-1)} + \sum_{m=1}^{\infty} \frac{(-1)^m}{m!} (1/2) \dots (3/2 - m) \frac{1}{3/2 - m - 1/(q-1)}. \quad (21)$$

In terms of the critical temperature T_c the correlation length ξ for high temperatures is given by the expression

$$\frac{1}{\xi} = 2\sqrt{\frac{\pi}{q-1}} \left(\frac{\langle n \rangle}{G_{3/2}(1, q)} \right)^{1/3} \left(\frac{T}{T_c} \right)^{1/2} \left[-1 + \left(\frac{-2}{\sqrt{\pi} G_{3/2}(1, q) (q-1)^{3/2}} \left(\frac{T}{T_c} \right)^{3/2} S_2(q) \right)^{2(q-1)/(5-3q)} \right]^{1/2}, \quad (22)$$

where the function $G_{3/2}(z=1, q)$ was calculated in Ref. [9]. In particular $G_{3/2}(1, 1) = 2.612$ and $G_{3/2}(1, q)$ increases with the value of q . A simple inspection shows that the correlation length ξ is smaller than the correlation length for the standard Bose-Einstein case ξ^{BE}

$$\frac{1}{\xi^{BE}} = 2\sqrt{\pi} \left(\frac{\langle n \rangle}{2.612} \right)^{1/3} \left(\frac{T}{T_c^{BE}} \right)^{1/2} \ln^{1/2} \left[2.612 (T/T_c^{BE})^{3/2} \right], \quad (23)$$

where $T_c < T_c^{BE}$. Figure 1 shows a comparison between these two functions for several values of the parameter q . Clearly, the correlation function decreases more rapidly as q increases from the standard value $q = 1$. At the critical temperature, $\xi \rightarrow \infty$ and the correlations become

$$G_c(\mathbf{R}) \approx \frac{1}{R\lambda_c^2}, \quad (24)$$

which, due to the inequality $\lambda_c > \lambda_c^{BE}$, is smaller than G_c^{BE} . Figure 2 shows α for $T \geq T_{critical}$ and some values of q in comparison to the $q = 1$ case. Since, at $T > T_c$, α is smaller for $q = 1$ we find that the correlation function for all temperatures is larger for the $q = 1$ case.

B. Critical behavior

In order to study the behavior at the critical temperature we need to expand the function

$$G_{3/2}(z, q) = \frac{2}{\sqrt{\pi}(q-1)^{3/2}} \int_0^\infty \frac{y^{1/2}}{[1 + y - (q-1) \ln z]^{1/(q-1)} - 1} dy, \quad (25)$$

in powers of α . It is clear from the previous discussion that $G_{3/2}(z, q)$ becomes the well known Bose-Einstein function $g_{3/2}(z)$ in the limit $q \rightarrow 1$. For these purposes we apply the same method used in Ref. [14], which gives a power series of α by performing first a Mellin transformation of the function and then applying the corresponding inverse transform. The Mellin transform of $G_{3/2}(z, q)$ is given by the equation

$$\begin{aligned} F_{3/2}(s) &= \int_0^\infty G_{3/2}(z, q) \alpha^{s-1} d\alpha, \\ &= \frac{\Gamma(s)}{(q-1)^{3/2+s}} \sum_{m=1}^\infty \frac{\Gamma(m/(q-1) - (3/2) - s)}{\Gamma(m/(q-1))}, \end{aligned} \quad (26)$$

and the inverse transformation

$$G_{3/2}(z, q) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{1}{(q-1)^{3/2+s}} \Gamma(s) \sum_{m=1}^\infty \frac{\Gamma(m/(q-1) - (3/2) - s)}{\Gamma(m/(q-1))} \alpha^{-s} ds, \quad (27)$$

where the contour of integration closes on the left half plane. With use of the approximation [15]

$$\frac{\Gamma(m/(q-1) - (3/2) - s)}{\Gamma(m/(q-1))} = \frac{1}{(m/(q-1))^{3/2+s}} \left[1 + \frac{b}{m/(q-1)} + \frac{c}{(m/(q-1))^2} + \dots \right], \quad (28)$$

with the constants

$$\begin{aligned} b &= \frac{1}{2}(3/2 + s)(3/2 + s + 1), \\ c &= \frac{1}{12} \frac{\Gamma(-3/2 - s + 1)}{\Gamma(3)\Gamma(-3/2 - s - 1)} (3(5/2 + s)^2 + s + 1/2), \end{aligned} \quad (29)$$

the function $G_{3/2}(z, q)$ is written

$$\begin{aligned} G_{3/2}(z, q) &= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{\Gamma(s)\alpha^{-s}}{(q-1)^{3/2+s}} \left[(q-1)^{3/2+s} \zeta(3/2 + s) + b(q-1)^{5/2+s} \zeta(5/2 + s) \right. \\ &\quad \left. + c(q-1)^{7/2+s} \zeta(7/2 + s) + \dots \right] ds. \end{aligned} \quad (30)$$

The function $\Gamma(s)$ has simple poles at $s = -n$ with residues $(-1)^n/n!$ and the zeta function $\zeta(w)$ has a simple pole at $w = 1$ with residue equal to $+1$. With use of the residue theorem the function $G_{3/2}(z, q)$ is expressed as a power series of α as follows

$$G_{3/2}(z, q) = \frac{1}{(q-1)^{3/2}} \sum_{m=1} \sum_{n=0} \frac{(-\alpha(q-1))^n}{n!} \frac{\Gamma(m/(q-1) - 3/2 + n)}{\Gamma(m/(q-1))} + \Gamma(-1/2)\alpha^{1/2} - \frac{1}{6}(q-1)^2\Gamma(-5/2)\alpha^{5/2} + O(\alpha^{7/2}). \quad (31)$$

A simple check shows that the series with integer powers of α reduces, as $q \rightarrow 1$, to the result in Ref. [14] $\sum_{n=0} (-\alpha)^n \zeta(3/2 - n)/n!$. At lowest order in α we obtain

$$G_{3/2}(z, q) \approx \frac{1}{(q-1)^{3/2}} \sum_{m=1} \frac{\Gamma(m/(q-1) - 3/2)}{\Gamma(m/(q-1))} + \Gamma(-1/2)\alpha^{1/2}. \quad (32)$$

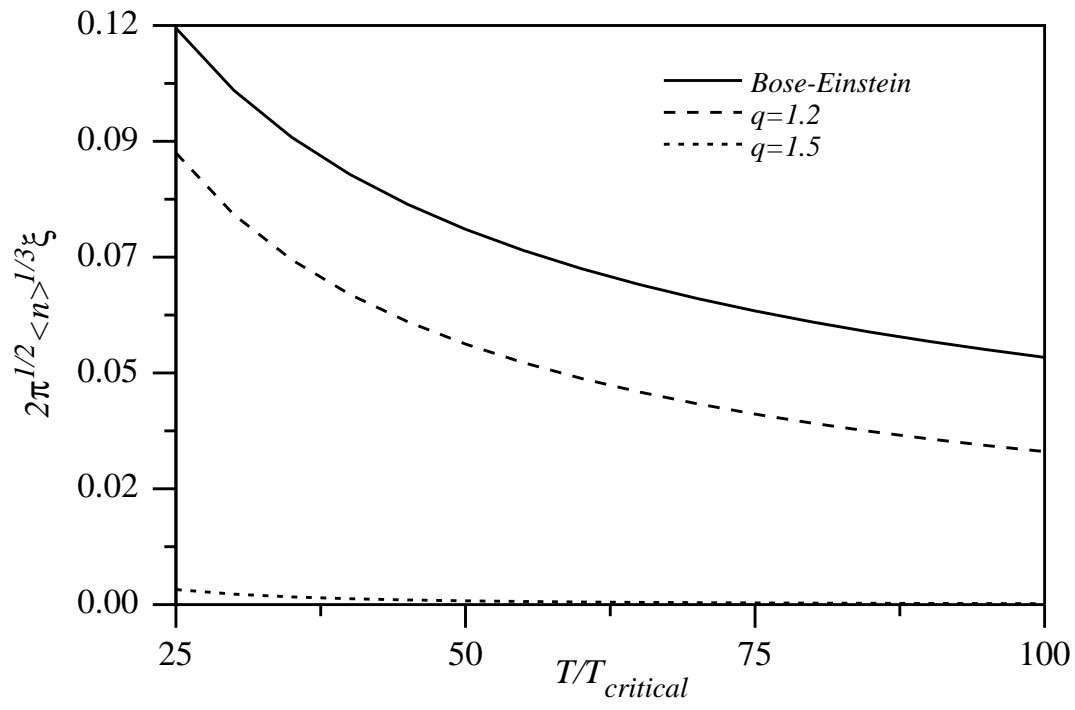
The series in equation (32) approximates at lowest order to the function $\zeta(3/2)$ and the last term is identical to the standard, $q = 1$, result. Therefore, since for $\alpha \approx 0$ we have $G_{3/2}(z, q) \approx \alpha^{1/2}$, defining $t = (T - T_c)/T_c$ we find that $\alpha \sim t^2$. In addition, the correlation length $\xi \sim \lambda t^{-1}$, as the standard case. Since, near the critical temperature, the t dependence of the functions $G_\nu(z, q)$ is the same as the case of the Bose-Einstein functions $g_\nu(z)$ and the thermodynamic functions of the two systems have the same functional form in terms of G_ν and g_ν , the remaining critical exponents are also independent of q .

III. CONCLUSIONS

In this paper our main concern has been to study the long range behavior predicted by thermodynamical systems described by a factorized partition function. As pointed out in the Introduction, this factorized partition function has been shown to approximate well the partition function of nonextensive statistics. A calculation of the correlation functions indicate that a Bose gas for the $q \neq 1$ case is less correlated than for $q = 1$. In particular, we showed that the correlation length for $q = 1$ is larger than for $q \neq 1$ at all temperatures, and the critical exponents are

independent of q . Certainly, our calculations can draw conclusions on the long range behavior of a thermodynamical system in the factorization approach only. On the other hand, correlations in nonextensive thermodynamics should be studied with use of the Tsallis' partition function. The fact that a Bose-Einstein gas obeying the studied factorized partition function is less correlated than for the Boltzmann-Gibbs case implies that the long range behavior expected in nonextensive thermodynamics is lost when the Tsallis' partition function is replaced by a factorized one. Thus, our results point out that the errors introduced by forcing factorization, which could be not significant for the evaluation of thermodynamic functions, are large enough that the long range behavior of Tsallis thermostatics cannot be studied within this factorization approach.

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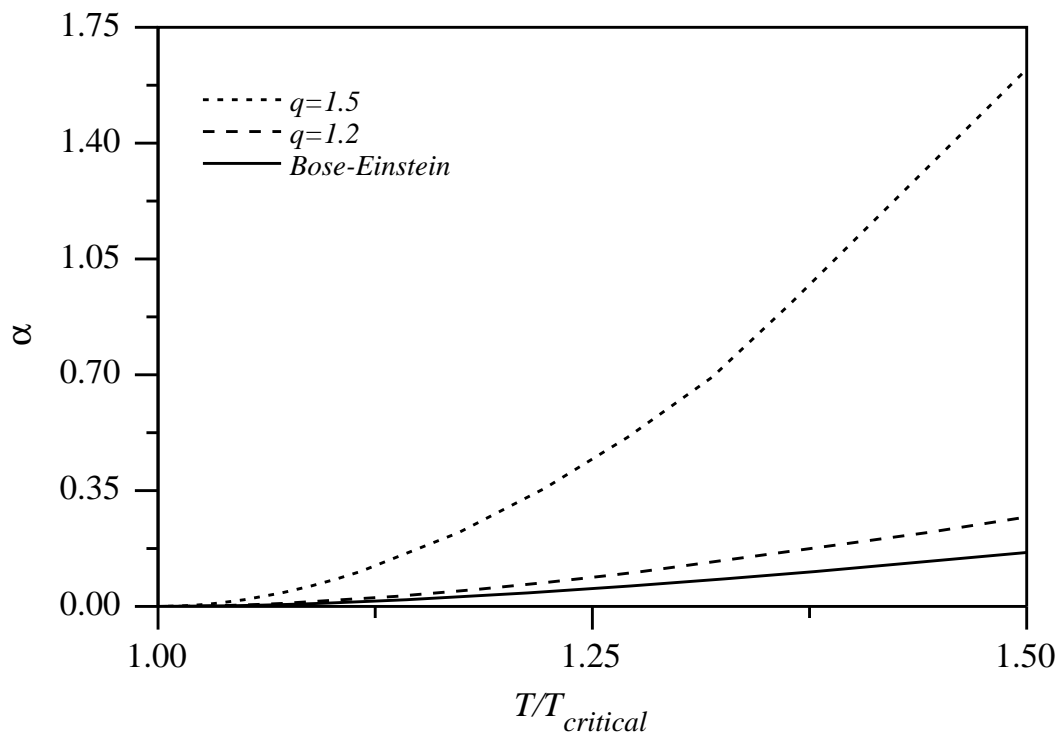


FIG. 1. The function $f = 2\pi^{1/2}\langle n \rangle^{1/3}\xi$, where $\langle n \rangle$ is the average number of particles per volume and ξ is the correlation length at high temperatures for the cases of $q = 1, 6/5, 3/2$ as a function of $T/T_{critical}$. $T_{critical}$ refers to the critical temperature for each value of q . This graph shows that the correlation length decreases as the value of q increases.

FIG. 2. The behavior of $\alpha = -\beta\mu$ as a function of the temperature for the cases $q = 1, 6/5, 3/2$, indicating that for low temperatures a Bose-Einstein gas is more strongly correlated for $q = 1$.